Cellular Automata, Modeling, and Computation

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(about 9800 words)

1. Introduction

Cellular Automata (CA) based simulations are widely used in a great variety of domains, from statistical physics to social science. They allow for spectacular displays and numerical predictions. Are they for all that a revolutionary modeling tool, allowing for "direct simulation" (Morgan and Morrison 1999, 29), or for the simulation of "the phenomenon itself" (Fox Keller 2003)? Or are they merely models of " a phenomenological nature rather than of a fundamental one" (Rohrlich 1990, section 10)? How do they compare to other modeling techniques?

In order to answer these questions, we present a systematic exploration of CA's various uses. We first describe their most general characteristics (section 2); we then present several examples of what is done with CA nowadays (section 3); we draw some philosophical implications from these examples (section 4) and finally draw some lessons about CA, modeling and computation.

2. What are cellular automata?

CA are employed in a variety of modeling contexts. As for other mathematical modeling tools, their modeling capacities are grounded in their mathematical properties; however, discussions about CA tend not to clearly distinguish between their purely mathematical properties and their representational and computational potential when they are used in modeling situations. However, in order to understand what CA contribute to the practice of modeling and simulation, CA have first to be described for themselves.

In this section, we describe the general properties of CA: first the mathematical, logical and computational ones, then the striking visual displays they allow for. We finally discuss the questions raised by the implementation of these formal structures.

2.1 The mathematics of CA

A cellular automaton consists in a dynamical rule which updates synchronously a discrete variable, defined on the sites (cells) of a *d*-dimensional lattice. The values s_l of the observable are taken in a finite set. The same (local) transition rule applies to all cells uniformly and simultaneously. CA rules can be expressed in the language used to study dynamical systems (Badii and Politi 1997, 49). An assignment of states to all cells is a *configuration*. A CA is *invertible* (or *reversible*) if every configuration has exactly one predecessor.

Different types of neighborhood can be defined. In a *von Neumann* neighborhood, cells to the north, south, east and west of the centre cell are defined as neighbors. The centre cell has 5 neighbors in total. A *Moore* neighborhood also includes diagonal cells to the northeast, northwest, southeast and southwest.

From the mathematical point of view, CA are an important class of objects that can be, and are, explored for themselves as well as applied to the study of natural phenomena. They behave differently from smooth dynamical systems, since the existence of discontinuities in arbitrarily small intervals prevents any linearization of the dynamics and, in turn, a simple investigation of the stability properties of the trajectories (Badii and Politi, 1997, 49-50). Nonetheless, some of the tools used to describe and classify discrete-time maps can be extended to CA; in particular the systematic study of recurrent configurations, because they characterize the asymptotic time evolution.

Noninvertible CA are of special interest for the study of complex systems. When acting on a seed consisting of a uniform background of equal symbols except a few (possibly one), some noninvertible CA are able to yield interesting limit patterns, neither periodic nor completely disordered.

Attempts to classify the variety of CA as discrete dynamical systems have been made. Wolfram has proposed to distinguish between four classes according to CA's behaviors; however, this "phenomenological" classification suffers from serious drawbacks. In particular, Culik and Yu (1988) have shown that it cannot be decided whether all finite configurations of a given CA become quiescent and therefore to which class it belongs. Other classifications have been proposed. For example, Langton (1990) suggests that CA rules can be parameterized by his λ parameter, which measures the fraction of non-quiescence rule table entries. Dubacq et al. (2001) as well as Goldenfeld and Israeli (2006) have also proposed a parameterization of CA rules as measured by their Kolmogorov complexity.

Traditional tools of statistical physics have also been used to study CA. For example, Chapman-Enskog expansions have been used to derive CA macroscopic laws or dynamics (cf. section 3.5). Renormalization techniques have also been used to characterize their macro-dynamics. The resulting map is in some sense an analogue of the familiar renormalization group flow diagrams from statistical mechanics, displaying stable fixed points (Goldenfeld and Israeli 2006). Symbolic dynamics, as well as the study of Lyaponouv exponents, entropy measures and fractal dimensions are also used (for a review of all this techniques, see Badii and Politi (1997, 54-55), Ilachinsky, 167-225).

The purely mathematical study of CA by various means is thus a growing field, still full of open questions, but whose results are already impressive. Here is Toffoli's and Margolus' bold appraisal of the importance of this field: CA are "abstract dynamical systems that play a role in discrete mathematics comparable to that played by partial differential equations in the mathematics of the continuum" (Toffoli and Margolus 1990, 229). We suspend our judgment about the validity of this claim for mathematics; nevertheless, we explore its implications for modeling in section 4.

As it is well-known, CA are not only interesting objects from a mathematical point of view, but also from a computer-scientific one. A CA can indeed be seen as "an indefinitely extended network of trivially small, identical, uniformly connected, and synchronously clocked digital computers" (Toffoli and Margolus 1990, 229). The notion of computation involved in these sentences is a large one. At least two notions of computation are currently used in papers about CA. According to the first one, "to compute" means "to be a universal computer in the standard Turing machine sense." A computer in this sense can simulate the architecture of any other sequential machine. This notion of simulation is a purely computer-scientific one. The second, less rigorous notion of computation involves a larger notion of simulation: "to compute" means "for any given mathematical situation, to find the minimum cellular space that can do a simulation of it". We insist that these two notions, albeit widely used, should not be mixed up and that only the first one can be rigorously defined.

Generally speaking, CA can be viewed as models of distributed dynamical systems (Toffoli 1984). They thus appear as a paradigm of distributed computation. In addition, it can be noted that invertible CA can perform reversible, namely information preserving, computing processes.

2.2 A striking format

When looking at Conway's Game of Life (see section 3.2) or at a simulation of car traffic inspired by Nagel's and Shereckenberg's models, or more simply at Wolfram's best-seller *A New Kind of Science* (2002), what is most striking is certainly not the mathematical properties of CA but rather the visual displays they permit. From the mathematical point of view, the visualization capacities of CA are inessential; however, for the human visual apparatus, they are of importance. When a CA based simulation is displayed on a computer screen, the human eye is prone to easily interpret what is going on to the extent that some clues are given to the viewer about what is represented and how. For example, CA based 2D simulations of forest fires are seemingly easy to interpret: since we are already familiar with this type of simulation, it is hardly necessary to look at the caption to understand how the represented fire propagates. The specific format of CA based 2D simulations (a 2D grid the cells of which can take at least two possible colors) allows for easy to grasp representation conventions.

From the "in principle" point of view criticized in Humphreys (2004), visual displays are not a respectful enough object of reflection for philosophy of science. However, Humphreys insists on the growing role visualization techniques play in today science. These techniques, which are massively used in all types of computer simulations, could not be dispensed with in the study of complex phenomena. Consequently, from the "in practice" point of view, the visualization capacities of CA are liable to the same analysis Humphreys (2004, 11-114) proposes for classical computer simulations.

2.3 Questions of implementation

In the same way as the mathematical and computation properties of CA have to be carefully distinguished from their visualization capacities, these properties should also be put apart from questions about the implementation of these logical machines. CA can be implemented on digital (sequential) machines as well as on parallel machines. In some cases the architecture of the machine can be the same as the architecture of the CA itself, namely, the nearest-neighbor-connected cellular space can be imaged directly in hardware. In this case the computation of a CA's evolution is obviously much faster.

As Margolus (1999) emphasizes, there is a serious mismatch on conventional, digital machines between hardware and algorithms when CA based simulations are run. When models are designed to fit CA computational potential, but are implemented on digital machines, the advantage of the uniformity and locality of CA systems is lost. Toffoli and Margolus designed and concretely built up several generations of CA machines (see the narrative of these attempts in Margolus 1999, and the technical details in Margolus 1996); however, "crystalline" hardwares are still in their infancy. Construction costs are still high.

3. Brief case studies

In this section, we briefly present some typical examples of what can be done with CA, which, taken together, are representative of today's research about CA - however we do not claim that they cover every aspect of it. Our main goal is to show that the philosophical questions CA raise depend on the scientific research programmes they are involved in and on what is expected from them in these programmes. The philosophical discourse about CA should reflect this variety, as we show in section 4.

3.1 CA as universal computers

Our first example of the various ways CA are used nowadays has already been briefly described in section 2.1: invertible CA can be used as parallel computers. They can perform elementary logical operations in a variety of ways and are on a par with Turing and RAM machines as abstract universal models of computation. According to Toffoli and Margolus (1990), invertible CA are even, these days, of significance comparable to the introduction of Turing machines (and similar paradigms of effective computation) in the late 1930s. If Toffoli and Margolus are right, the importance of CA for the entire domain of theoretical computer science cannot be overestimated. They could allow for new, unexpected insights into the nature of computation.

Let us continue Toffoli's and Margolus' comparison between Turing machines and invertible CA. Turing machines are the product of the tentative "to capture, in axiomatic form, those aspects of physical reality that are most relevant to computation". By comparison, CA are, according to Toffoli and Margolus, "more expressive" than Turing machines, "in so far as they provide explicit means for modeling parallel computation on spatio-temporal background". Toffoli and Margolus have further explored the computing potential of CA. For instance, in their (1990), they explore the following question: "How does one tell if a CA is invertible?". Theorems has been demonstrated about the existence of effective procedures for deciding whether certain types of CA are invertible or not. They also examine how one can make a CA rule invertible. All these investigations shed light on a way of being a universal computer that is completely different from being a Turing machine.

By way of conclusion about this first example, we attempt at clarifying (and criticizing) a maybe surprising parlance of Margolus and Toffoli, who claim that invertible CA can "model" parallel computation. Other possible choices to express the same idea are "simulate" or "emulate". Toffoli's and Margolus' vocabulary indicates that their notion of modeling has a very large extension. We insist that this sense of "modeling" is completely different from the usual sense, as in the expression "modeling car traffic", for instance. When CA are said to "model" parallel simulation, no representation of any phenomenon is involved: there is no CA being "about" parallel computation. We prefer to say that CA just *perform* parallel computation. In the remainder of this paper, we will be careful to reserve the term “model” to representations of phenomena since we believe that it helps keeping distinct problems clearly separated. Toffoli’s and Margolus’ way of speaking reveals that CA are involved in a tricky set of questions about representation, computation, and mathematical formalism. We aim at clarifying this nub of problems in presenting other examples in which CA play other roles.

3.2 “Life”

Conway’s “Game of Life” is perhaps the most widely known CA rule (Berlekamp et al. 1982). It involves a 2D square lattice with one bit at each lattice site, and a non-invertible rule for updating each site that depends on the total number of 1’s present in its eight nearest neighboring sites. If the total of its neighbors is 3, a given site becomes a 1, if the total is 2, the site remains unchanged; in all other cases the site becomes a 0.

When the initial state is a random distribution of 0s and 1s, and when the Life dynamics is run at video rates, we can observe a lively pattern of activity, with small-period oscillating structures, various stable configurations and periodic patterns, gliders (if the initial configuration is well-chosen), etc. Some population of cells can grow indefinitely. Some configurations move through the lattice and leave “wreckage” behind.

What is most striking with Life is that despite the simplicity of its rule, it can exhibit a wealth of complex phenomena. As the most successful achievements of Artificial Life at its beginning, Life is an example of a use of CA governed by the following question: What are the most basic mechanisms generating evolving complex phenomena, comparable to those exhibited by the evolution of life on Earth? This investigation is carried on by exploring the universes generated by the Life rule. The same type of investigation is also carried on in the fields of genetic algorithms (Holland, 1975) and multi-agent systems. It can be compared with the attempts that lead last century mathematicians to look for the basic operations that are needed to compute all functions that were currently computed by hand; this gave birth to what is now known as Turing machines, lambda calculus or recursive function theory.

3.3 The Billiard Ball Model Cellular Automaton

The Billiard Ball Model Cellular Automaton (BBMCA) is a purely digital model of computation which is closely related to a continuous model of computation, Fredkin’s Billiard Ball Model or BBM (Fredkin and Toffoli 1982). The BBM is a continuous dynamical system whose initial conditions are suitably restricted and whose evolution is observed at regularly spaced time intervals only. Due to these restrictions, it can compute logical operations. The BBMCA is a CA whose behavior is the same as the original BBM: it is also a universal computer.

The BBM is a 2D gas of identical hard spheres to which the following convention is associated: if the center of a sphere is at a given point in space at a given point in time, we say here is a 1 there, otherwise there is a 0. The1s can move from place to place. The number of 1s is constant. Here is the link between hard spheres and logic: every place where a collision might occur is viewed as a Boolean logical operation. This implies that the angle and timing of the collisions and the relative speeds of the balls have to be precisely controlled. Moreover, mirrors are used in order to route and delay balls (that is, signals) as required in order to perform logical computation.

When a BBM is only observed at integer time-steps, it appears as a squared lattice of points, each of which may be black or white (or assigned a 0 or a 1), evolving according to a local rule. The construction of a CA having the same behavior as the BBM thus looks like an easy task. As Margolus (1984) emphasizes, it is not so easy, since a direct translation would require a complicated set up (with 6 states per cell, for instance). However, BBMCA do exist and are universal computers in the same way as BBM are. The trick is to design two ways to group cells into blocks and apply the rule alternatively to the even and odd 2×2 blockings (Margolus 1984, 88-89; 1999, 16). To put it another way, the balls in the CA are represented by spatially separated *pairs* of particles, one following the other—the leading edge of the ball followed by the trailing edge. (A particle in a BBMCA is just a block of 4 cells one of which is assigned a one.) Figure 1 represents a BBMCA collision (see legend for details).

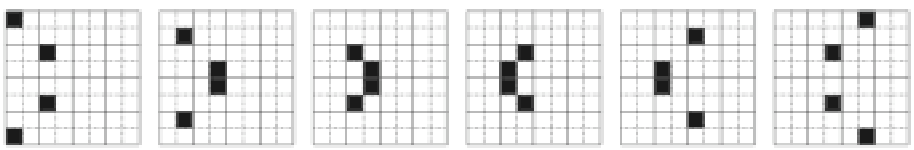

Figure 1. Successive snapshots of a small area where a collision is happening. In the first image, the solid-blocks are about to be updated. The blocking alternates in successive images. (Margolus 1999, figure 1.9)

The BBMCA is interesting neither as a computer *per se* nor as a classical mechanical model of collisions between hard spheres. However, as Margolus (1999) emphasizes, it is “a wonderful bridge between the tools and concepts of continuum mechanics, and the world of exact discrete information dynamics”. It can be used in investigations about connections between physics and computation. Moreover, it illustrates how CA can contribute to research in fields like the physic of information (Zurek 1984), for example to questions about entropy and reversibility of computational processes.

3.4 Exploration of the Ising model

Whereas Life does not follow from any mathematical representation of the evolution of life on Earth, but is rather designed to investigate its most basic features, other CA have been designed to investigate mathematical constructs, especially those involving a regular lattice structure and local dynamic rules, among them the *Ising model*, as well as models of percolation, nucleation, condensation, etc. (Vichniac 1984, 101). The Ising model surely has a physical origin; however, the purely mathematical investigations of its properties has developed of its own, and CA allow for interesting (albeit negative) on this road.

A strong motivation a CA based investigation of the Ising model is to try and save computational resources by using a computational architecture with local updates rules. The Ising models involves a lattice each site of which is associated a spin variable s_i, which can take two values, +1 or -1. The energy H of a given configuration S of spins is made up of two parts : (1) the contribution due to the interaction with an external field M, equal to $H_{S\_M} = - M \ {}_{\_i} \ {}_{\_i}$; (2) the contribution arising from the interactions between the spins, and equal to $H_{S\_S} = - J \ {}_{\_i,j} \ {}_{\_i} \ {}_{\_j}$. One then defines the partition function $Z = \ {}_{\_S} \ e^{- H(S) / k T}$., where k refers to the Boltzmann constant and T to the system’s temperature.

In the canonical ensemble, each configuration has probability $p(S)= e^{- H(S) / k T}. Z^{-1}$: it depends on the global value of the energy. In order to compute the average value of an observable, the trick of usual Monte Carlo simulations is to find out transition rules between configurations that enable one to create a list of configurations correctly sampling the canonical distribution and avoid computing Z. Vichniac tried to find out a CA rule sampling the canonical distribution. It turned out that it is not as simple a task as he hoped. In spite of a striking resemblance between CA and the Ising model, there is no obvious (topology conserving) simulation of the wandering of Ising configurations through the canonical ensemble with a simultaneous updating of *all* the spins at each interaction. Spurious stable maximal energy checkerboard patterns emerge and ruin the simulation.

Other investigations have nevertheless shown that there is a fundamental relationship between d-dimensional probabilistic CA (PCA) and (d+1)-dimensional Ising spin models. By averaging over all possible space-time “histories”, properties of the PCA such as correlation functions correspond to thermodynamics averages in the associated spin model. The link between the geometries of CA lattices and of Ising spin models is not as straightforward as one could have wished. For example, the time evolution of the one-dimensional probabilistic CA system is equivalent to the equilibrium statistical mechanics of a spin model on a triangular lattice (see Ilachinsky, 2001, pp. 343 sq. for a review and Domany and Kinzel, 1984, Georges and Doussal, 1989 for the original articles).

This example shows that the use of CA to investigate extended mathematical models is not straightforward. In the same time, it illustrates that deep relationship between CA and other extended model such as spin systems, neural networks or percolation models do exist, and are being investigated. This confirms again that CA are not a shining isolated star in the sky of mathematics (see section 2.1).

3.5 Lattice gas models

We have so far described several cases in which it was the mathematical properties of CA that were investigated and exploited within mathematical investigations. The potential of CA is not limited to computer science and mathematics, though. CA can also be attributed remarkable representational capacities and are investigated as such. We will review several cases in which this representational potential is successfully exploited and show that there is no single law governing the use of CA in modeling projects.

Our first example (lattice gas models) is drawn from a domain, hydrodynamics, where Navier-Stokes continuous equations had been unrivalled as a model for more than 100 years. This model has been studied both analytically and numerically in the second half of the 20th century. From the 1980s on, *lattice gas models* have been introduced for the study of fluids. Lattice gas models have been both calibrated (Humphreys, 2004, p. 117) by reference to many already known situations (Hasslacher, 1987) and used independently in new situations (Doolen, ed. 1991; Rothman and Zaleski 1997 Succi 2001; Wolf-Gladrow 2000).

A major motivation for the use of CA in modeling non-equilibrium fluid dynamic is that it avoids resorting to artificial (although common) idealization procedures. As Hasslacher (1987) puts it, the discretization of Navier-Stokes equations is equivalent to introducing an artificial microworld, with a particular microkinetics. The particular form of this microworld is fixed by mathematical considerations of elegance and efficiency which are applied both to simple arithmetical operations and to the particular architecture of available machines.

On the contrary, "discrete fluids", namely models of fluid dynamics using CA as their basic ingredients, do not contain, according to their proponents, any "artificial" components. In the simplest CA model in 2D, namely the hexagonal model, no transformations (discretization) of partial differential equations are necessary. Conservation of momentum and particle numbers are from the start built into *already exactly computable* collision rules. Together with collision rules and an exclusion principle (forbidding two particles to be at the same place at the same time), they do the job of reproducing the collective behavior predicted by the compressible and incompressible Navier-Stokes equations.

The geometry of the lattice is especially important. In order to see why, let us have a look at how the collective behavior of the particles is derived (*a*) in continuous models and (*b*) in Lattice Boltzmann Methods (LBM).

(*a*) Starting from an atomic picture and Newton's laws, we apply kinetic theory and obtain a probabilistic description of the motion of particles according to their positions and speeds (namely, their distribution in phase space). Then we come to Boltzmann Transport Equation, which describes how the probability distribution of the particles in the phase space evolves. The next step is to use appropriate approximations and Chapman-Enskog expansion and to compute the integrals[1] corresponding to the different conserved quantities. This is how Euler and Navier-Stokes equations are recovered, as well as tensors describing the fluid.

(*b*) One can check in exactly the same way that the same macroscopic Navier-Stokes-like behavior can obtain in a lattice gas (except that the derivation is made in a discrete phase-space). This derivation approach makes clearer how the macroscopic behavior of the fluid depends on the microscopic behavior of particles. The best example of that dependence is the derivation of the momentum stress tensor Π_{ij} describing and controlling the convective and viscous terms of the Euler and Navier-Stokes equations. This tensor must be isotropic (since fluid motions are isotropic). A square lattice does not contain enough symmetries for Π_{ij} to be isotropic; only a hexagonal lattice can do that in 2D. By using considerations on tensor structure for polygons and polyhedra in *d*-dimensional space, one can also arrive at satisfactory models in any dimension.

This example indicates *i*) that CA based simulation can successfully compete with more traditional approaches, even though it starting point is utterly different and *ii*) that the evolution of a CA used to represent the motion of a fluid can not be simply interpreted following the convention "one black cell – one particle". Such a convention would be completely misleading. The representational capacities of CA for modeling fluid dynamics are huge, but they are also hard to tame, and unpleasant surprises are not uncommon.

Let us conclude on this example with one of its most convincing proponents:

> "The methods we use to do this are very conservative from the point of view of recent work on cellular automata, but rather drastic compared to the approaches of standard mathematical physics. Presently, there is a large gap between these two viewpoints. The simulation of fluid dynamics by cellular automata shows that there are other complementary and powerful ways to model phenomena that would normally be the exclusive domain of partial differential equations." Hasslacher (p.177)

3.6 "Phenomenological" models of complex phenomena

The use of CA in modeling is not always associated with well-confirmed physical theories or comparable to other alternative models like in the previous example. CA based simulation can be designed independently of any underlying theories, but rather from just a few leading assumptions about the target phenomena. These models, for instance models of car traffic, of forest fires or of snow transport by wind, seem to have nothing in common, as far as the entities involved and their properties are concerned. However, the use of CA to study these phenomena reveals that well-known methods of statistical physics can be efficiently applied in those cases. For example, these models can be studied using mean-field approximation (Schadschneider and Schreckenberg, 1993) and dimensional analysis (Nagel and Schreckenberg, 1992). We briefly describe CA based models of car traffic in the following.

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[1] For example, you can have an equation describing the balance of energy in a region of phase space. By suitably integrating over phase space the two members of the equation, you get new macroscopic equations.

The first traffic flow model (Nagel and Schreckenberg 1992) is defined on a one dimensional array of L sites and with open or periodic boundary conditions. Each site is either occupied or empty and each cell is characterized by a value between 0 and v_{max}. The update rule is the following:
- acceleration by one velocity unit if the velocity of a vehicle is lower than v_{max} and if the distance to the next car ahead is larger than $v+1$
- if a vehicle at site i sees the next vehicle at site $i+j$ (with $j \leq v$), it reduces its speed to j-1
- randomization when stationary patterns occur
- each vehicle is advanced by v sites at each time step

This is just a short description of a probabilistic CA rule with a neighborhood of v_{max}+1 nearest neighbors . The terminology (“vehicle”, “sees”) is just a convenient way to describe a microscopic dynamics between particles characterized by a position and a speed on a discrete space with density as a varying variable. These basic properties are sufficient to obtain a phase transition from laminar flow to start-stop-waves, namely, to correctly predict traffic jams in given situations.

Additions to the original model have been made. For example, a two-lane model has been studied, as well as the effect of one-lane sudden bottleneck. Breaking or acceleration parameters can be refined by using empirical data in order to try and explain more refined phenomena such as average traffic in particular cities (Olmos and Munoz, 2004). These models can be studied using usual techniques of statistical physics such as mean-field approximation (Schadschneider and Schreckenberg, 1993) and dimensional analysis (Nagel and Schreckenberg, 1992).

Forest fires have been investigated with similar models. The interested readers can look at Bak, Chen, and Tang (1990), Chen, Bak, and Jensen (1990), Drossel and Schwabl (1992), Grassberger (2002), Henley (1989), Henley (1993).

What is striking in these models and other so-called “phenomenological” models is that whereas predictive power does not depend on any background theory, the phenomena so described exhibit macroscopic properties that are characteristic of other complex systems, like self-organization. Those properties are difficult to access to within other approaches of such phenomena.

3.7 Schelling model

Schelling model (1969, 1971) has been proposed to study segregation effects. The representational framework of Schelling model is the following: individuals belong to two different classes, black and white or, in more abstract terms, stars and zeros. Each individual is represented to interact with its neighbors according to the Moore neighborhood pattern and is attributed migration options, allowing for the definition of a local rule. An individuals leaves its actual neighborhood if it does not have a required minimum frequency of individuals of its own class. For instance, individuals might wish to live in a neighborhood where their class is not in a minority. If that requirement is not met, an individual will move to the nearest alternative site where it is. This rule evolves in such a way as to allow for neat segregation effects (see examples in Hegselmann and Flache1998), corresponding to observations in certain cities.

The main question about such models is whether they are really capable of a faithful representation of collective behavior of human beings in spite of the minimalism of their assumptions (encapsulated in the local rule). Can human behavior be reduced to such a simplistic representation? The empirical success of Schelling model and its developments seems to show that populations of human beings exhibit behaviors liable of a statistical-mechanical description. However, taking it seriously is at odds with many psychological and sociological theories according to which much more complex elements are involved in the explanation of human behavior. These theories would not consider as appropriate that statistical-mechanical mechanisms have any relevance to understanding human behavior.

By contrast, Hegselmann and Flache (1998) claim that CA based models cover basic features of a significant class of social processes, those based on the fact that over a period of time numerous people locally interact and that the neighborhoods of interaction overlap. Moreover, CA based models of some social phenomena make it quite clear how certain macro effects are dynamic consequences of decisions and mechanisms operating only at the micro level. Order, structure, clustering and segregation are all generated by such micro level rules. Hegselmann and Flache (1998) also emphasize that CA based modeling is not always simplistic: it is flexible enough to allow for various (narrow or wide) definitions of locality and allows for investigations in social self-organization and corresponding political or economic manifestations based on the “invisible hand” paradigm. According to that paradigm, individuals acting in a more or less self-interested way will nevertheless produce desirable collective results on the macro level. CA based models of human behavior can thus be sufficiently enrich to answer fundamental question about societal organization (Epstein and Axtell 1996, Guenther *et al.* 1997).

3.8 Conclusion

The above examples show that CA are involved in a lot of distinct domains, from computer science and pure mathematics to the "phenomenological" study of complex phenomena, be they natural of social. Their striking mathematical and logical properties, as well as the powerful visualizations they allow for, should not hide the fact that in order to have them *represent* the evolution of natural or social systems, their particularities have to be carefully tamed and the various representational relationships they are involved in have to be no less carefully established.

The versatility of CA is comparable to other mathematical devices that have been used in mathematics and in modeling for a longer time, like differential equations or matrixes. Claims have been made, however, about the distinctive novelty CA are supposed to bring about in science (Rohrlich 1990, Hughes 1999, Fox Keller 2003). In the following section, we discuss these claims' legitimacy as well as the implications of the various uses of CA in modeling.

4. Implications for a philosophical analysis of CA based simulation

This section is focused on the representational capacities of CA: we examine how CA are used in various modeling and theoretical physics contexts, leaning on the examples in section 3. Modeling phenomena with CA obeys different constraints than modeling with partial differential equations (PDE). The general question in this context, according to Hasslacher (1987) is to find a minimal spatial structure enabling the implementation of Boolean operations and devise a (local) dynamics for it. In contrast to modeling with PDE, mathematics plays a lesser role than the building up of a rule enabling parallel Boolean operations.

This striking difference is uneasy to grasp because of the usual modeling habits relying on PDE. Is it enough to claim that modeling with CA is radically different from modeling with PDE? We claim that the computer-scientific tree should not hide the modeling forest. Modeling can be carried out in many different ways and by means of many different tools. From the modeler's point of view, using CA instead of PDE makes a huge difference; however, modeling, as a representational activity, is doomed to use any available means. Consequently, neither PDE nor CA are consubstantial to it, even in physics.

In order to investigate the relationships between the representational and the computational capacities of CA, we first examine whether CA based simulation can be called "direct" in any sense. We then make a point about the implication of "exact computation" as a oft-emphasized feature of CA models. In section 4.3 we compare CA models with other modeling device and assess the virtues of pluralism in modeling. We conclude section 4 by examining the potential role of CA for fundamental physics. Whereas CA shed light on many questions about modeling, we have chosen to only discuss a few points about the relationships between modeling and computation.

4.1 Can simulation be "direct"?

The reason why CA based simulations are sometimes said to be "direct" is mostly that some of them, for instance simulations of the growth of stars, of traffic flow, of forest fires, etc., do not rely as much on underlying theories as do other types of simulation, for instance simulations in hydrodynamics. "Direct" in this sense means "without any detour via a theory usually appealed to in the investigation of the given phenomena". In this section, we investigate what is involved in this claim.

The starting point of the relevant cases of CA based simulation is to determine basic local interactions responsible for the particularities of global behavior in each phenomenon and to try and represent them with a CA rule in order to obtain the same macro-particularities. The leading question in this enterprise is: "Are there well-established correspondence rules that I can use to translate features of the system I want to model into specifications for an adequate CA model of it?" (Toffoli and Margolus 1990). So, from a practical point of view, the problem is to provide an analysis of the studied phenomenon that be suitable for a CA based representation of it. There is no requirement that the correspondence rules be based on any already available explanatory theory. More precisely, the question of how one justifies the choice of to-be-represented features within the studied phenomena is an independent question. It can be asked as well for other types of models. In some cases, the justification of which CA rule is chosen may only be that it yields the right behavior. In other cases, the justification may be that one had good independent reasons to choose represent such or such features of the target system and the CA based model turns out to be successful for a wide range of predictions.

Consequently, in these examples of "phenomenological" models, no use is made of any explanatory theory; by contrast, in the traditional simulations of hydrodynamics, it is the explanatory theory, *i.e.*, Newtonian mechanics developed in Navier-Stokes equations, that is the basis of the implemented model. However, this does not imply that mechanisms revealed by the CA rule cannot be explanatory. In particular, CA can be useful to explore the set of behaviors characteristic of "universal physics", like phase transitions, critical phenomena, scale invariance, and the like (cf. Batterman 2002, 13). When phenomena exhibit universal properties, it may happen that the details of the true mechanisms do not matter. In those cases, CA models may capture the "right physics" (to use Batterman's expression), as lattice gases do, even if they are not literally exact.

It is thus clear that CA based simulation are not "purely phenomenological". As emphasized by Vichniac (1984), "CA do not only seek a mere numerical agreement with a physical system, but they attempt to match the simulated system's own structure, its topology, its symmetries, in short its 'deep' properties". CA based simulations being "direct" in the sense explicated above does not imply that they just reflect the surface of phenomena. On the contrary, they may reveal other important properties than the ones which are traditionally used in the modeling activity.

4.2 The virtues of pluralism in modeling

As manifest in our presentation of lattice gas models (section 3.5), different models, including CA based models, of the same phenomena can be built up. It is sometimes claimed that due to different models, one can represent different aspects of the same target system; however, in this case, the very same aspects are represented, in particular the relationships between micro-properties of particles and macro-properties of fluids. We do have genuine alternative models of fluids.

An objection might come to mind at this point. Are not LBM just numerical methods, rather than alternative models? This objection can be answered as follows. First, as we have seen, LBM models are not obtained from the numerical study of Navier-Stokes equations but obtained independently. They are obtained by taking into account conservation laws and deeper symmetries. Second, lattice gases and LBM require much more physical theory than pure numerical methods do. Whereas one can teach to a beginner how to apply finite-difference schemes within a few hours, LBM require physicists to fully understand statistical mechanics and to have deep insights into the significance of symmetries, in particular when spurious invariants have to be detected and destroyed (for example three-particle collisions in FHP) or when consequences of missing symmetries have to be scaled away (for example violations of Galilean invariance).

The differences between models governed by Navier-Stokes equations and Lattice Boltzmann Methods are nevertheless important. Here are some about prediction, representation, and computation.

- Lattice gas models are stable, where as in classical simulations of fluids dynamics the code may stop running because the algorithm becomes unstable.
- Energy and momentum are conserved exactly; no round off error can occur.
- Boundary conditions and particular geometries are easy to implement
- Every single bit of memory is used equally effectively (this has been called "bit democracy" by von Neumann), whereas in classical simulations every number requires a whole 64-bit word. All that one needs to know is whether or not a particle with a given velocity exists in a given cell. Only 6 bits of information are needed to completely specify the state of a cell. Consequently, there is no wasting of memory.
- Lattice gas operations are bit oriented vs. floating-point-number oriented, and are thus executed more naturally on a computer.
- The algorithm is inherently parallel.
- More complex models than the simple hexagonal model are required in order to get more accurate results. However, the computational price of enhanced accuracy may be high. The most important limitation of these models is that their efficiency is restricted to a certain range of flow velocities. It derives from the fact that all particles are given the same velocity.
- As the discreteness of the lattice gas introduces noise in the results, noise reduction is another tradeoff case of computational price vs. accuracy. There is no systematic procedure for noise reduction. Noise is surely a problem; however, it also ensures that only robust (namely, physical) singularities survive, whereas in standard codes, which produce less noise, mathematical artifacts can produce singularities.
- Finally, the cognitive cost of switching from PDE to CA is difficult to evaluate. As noted above, understanding the basic operations is easy, but a deeper understanding requires some deep insight into more fundamental physics.

Are discrete fluids redundant with respect to classical models? They allow physicists to obtain about the same results. However, they shed a new light of the mathematical physics of fluid dynamics. When exploring the class of functionally equivalent models, namely those models with different geometries and rules that produce the same dynamics in the same parameter change, important features are revealed about the mechanisms responsible for the qualitative features of hydrodynamics. Robust mechanisms appear more clearly. Overall, as noted by Wolf-Gladrow (2000, 245-246), complementarity, rather than competition, is on the agenda of hydrodynamics.

4.3 What does "exact computation" mean?

In one of the first reflexive study about CA based simulation, Vichniac (1984) proposes to add a third alternative to the classical dichotomy between models that are solvable exactly (by analytical means) but are very stylized and models that are more realistic but can be solved approximately (by numerical means) only. According to him, certain CA models can be put in the class of "exactly computable models", for they have enough expressive power to represent phenomena of arbitrary complexity and at the same time can be simulated exactly by concrete computational means. In these CA models, the mathematics is exactly implemented and is thus automatically free of numerical noise. These models are not built up to solve any equations. They merely perform simple space-dependent decisions. Consequently, according to Vichniac, they are capable of digital non-numerical simulations of physical phenomena.

Are thus CA models a panacea for all problems of round-off errors, divergence, tractability of discretization techniques, etc., that are usually encountered in traditional simulations? As indicated above, in order for a CA model to fill its role, a careful analysis of the studied phenomenon has to be made that should match the model. Exact computability associated with satisfactory representational ability cannot be the property of any CA model: exact computability is at best an interesting by product of a well designed model. However, once adequate "correspondence rules" have been designed, exact computation is of course invaluable.

Exploring the effects the advance of our knowledge of CA may have on the very nature of mathematical physics, Toffoli (1984) claims that our new knowledge of CA opens the possibility to replace the customary concepts of real variables, continuity, etc., with more constructive "physically-minded" counterparts. The success of differential equations as a starting point for modeling and simulation in physics depends, according to Toffoli , on the choice of symbolic integration as a main instrument of our understanding of natural processes. Once this choice has been given up, on the ground that few differential equations have a closed-form solution, there is no reason to keep differential equations as the starting point for modeling.

Differential equations are numerical computed (for instance on general-purpose computers) in a manner that is "at least three levels removed from the physical phenomena that they aim at representing: (a) we *stylize* physics into differential equations, then (b) we force these equations into the mould of discrete space and time and truncate the resulting power series, so as to arrive at *finite-difference equations*, and finally, in order to commit the latter to algorithms, (c) we project real-valued variables onto finite computer words ("round-off"). At the end of the chain we find the computer – again a physical system". This analysis leads Toffoli to ask whether there could be "a less roundabout way to make nature model itself?" (Toffoli 1984, 121).

Toffoli outlines an approach where the theoretical mathematical apparatus in which one "writes" the models is essentially isomorphic with the concrete computational apparatus in which one "runs" them. Starting from this approach, the few infinities that one may still want to incorporate in a physical theory (e.g., as the size of a system grows without bounds) are defined as usual by means of the limit concept. However, in this approach the natural topology in which to take this limit is that of the *Cantor set*, rather than that of the real numbers. (117-118).

Toffoli's proposal goes very far on the road of the possible effects of exact computability of CA models on physical modeling. Whereas this approach still remains partly speculative, some important results have been achieved (cf. Chopard and Droz 1998). For the time being, exact computability should not overshadow the fact that CA models are delicate constructs whose computational capacities are sometimes difficult to tame – as is any model using sophisticated mathematics.

4.4 A new kind of physics?

In his 1982 paper, Feynman asked whether "nature, at some extremely microscopic scale, operates exactly like discrete computer-logic". He then expressed the guiding line of the (supposedly) new kind of physics that CA make possible: "So I have often made the hypothesis that ultimately physics will not require a mathematical statement, that in the end the machinery will be revealed, and the laws will turn out to be simple, like the checker board with all its apparent complexities". This hypothesis has been further developed by Wolfram, Fredkin, Finkelstein, Minsky, Wheeler, Vichniac and Margolus. It had previously been discussed by Konrad Zuse (see Fredkin 1992 for a review).

Vichniac (1984) characterizes this trend of thought as a "bold approach, in line with the atomistic tradition that advocates taking discreteness seriously", that "sees nature as locally – and digitally – computing its immediate future". According to Fredkin, the core of the hypothesis is that we assume that there will be found a single CA rule that models all of microscopic physics, and models it exactly. The general hypothesis of "crystalline computation" (Margolus' phrase), according to which CA might be the formalism of a new, discrete and more faithful physics, is still (almost) purely speculative. Nevertheless, briefly presenting it may help get a better understanding of the potential of CA in terms of fundamental physics and draw a clear distinction between what is speculative and what is not about CA.

According to Margolus, the hypothesis is that crystalline arrays of logic, namely CA, might be able to simulate our known laws of physics "in a direct fashion" (1999). There is some ambiguity in this expression; however, it may be understood as meaning that using CA to do fundamental physics would prevent us from the idealizations and approximations that are indispensable when other formalisms are used. The main claim of the proponents of crystalline computation or digital mechanics is that:
(1) CA may be a better mathematical machinery than continuous differential equations for describing fundamental physics dynamics.

The main motivation for (1) is that CA allow for exact models. "Exact" means that no approximations are required. Every discrete formalism is exact in this sense. However, an exact computation may be performed within a highly idealized representation. Exactness of computation is thus not all what there is to "direct simulation". A second claim is contained in the "crystalline computation" hypothesis , namely
(2) CA can represent fundamental laws of physics without using any idealization.
The "crystalline computation" hypothesis is therefore a hypothesis about the *representational* capacities of CA as well as about their *computational* capacities. Toffoli and Margolus (1990) thus insist that invertible CA are playing an increasingly important role as *conceptual tools* for theoretical physics.

The main argument in favor of claim (2) is that "the most essential property of CA is that they emulate the spatial locality of physical law" (Margolus, 1999). "Spatial locality" means that no action-at-a-distance is allowed. The spatial locality of CA is as follows. CA computation can be viewed as a regular space-time crystal of processing events, namely a regular pattern of communication and logic events that is repeated in space and in time (Margolus, 1999). Of course, the patterns of data that evolve within the computer are not necessarily regular, only the structure of the computer is. It seems to be a safe bet to claim that the fundamental laws of physics are local in this sense. Nevertheless, Margolus' sentence is ambiguous, since neither the intended meaning of "emulation" nor the implication of CA emulating spatial locality is clear.

In their 1990 paper, Toffoli and Margolus also insist on the uniformity of CA laws as an argument in favor of claim (2). Uniformity, according to which the laws of physics are the same at every instant of time, is another fundamental aspects of the laws of physics. Other properties of CA also justify claim (2) according to Margolus (1999), namely their ability to represent energy conservation, invertibility, and the possibility that classical bits capture the finite-state character of a quantum spin system. Margolus thus claims that CA allow one to simultaneously capture several basic aspects of physics in an exact digital model.

Toffoli and Margolus (1990) conclude from the arguments they give in favor of claim (2) above that a "strong effectiveness is built in the definition of CA" and argue that continuous dynamical systems make up a weaker standard for effectiveness. Fredkin emphasizes that it is possible to map properties of a RUCA informational process onto properties of physics (energy, angular momentum) and have those properties conserved as a consequence of the reversible rule.

Claims (1) and (3) are linked together by a further one according to which
(3) "Exactly the same general constraints that we impose on our CA systems to make them more like physics also make them more efficiently realizable as physical devices" (Margolus, 1999).
This third claim is about realizability or implementation of CA computation. According to it, the fundamental laws of physics are the very laws of efficient computation.

5. A modeling tool among others

The examples in section 3 as well as the discussion in section 4 make clear that CA are neither revolutionary discovery capable of solving every problem nor just some odd mathematical trick that should not be paid attention to from a philosophy of science point of view. We have shown that CA are first and foremost a mathematical tool among others. Partial differential equations, stochastic systems and matrices are other such tools.

As such a mathematical tool, CA can be expected to be well-suited to some tasks and less to others; however, this cannot be predicted before trying. PDE proved to be a particular powerful and easy-to-handle tool during the last centuries. CA may prove just as useful in the future. As we have emphasized in this paper, there are already entire domains and types of phenomena about which CA do better than traditional models (or computer architectures). In the study of phenomena in which stability matters a lot, CA fare better from a representational or predictive point of view. This implies that CA cannot be viewed only as a numerical trick only useful to speed up calculations. Nonetheless, CA can above all be helpful regarding computational issues, in every case where parallel computation is faster than sequential computation. Many more systems involving local interactions may soon fall within this category. As illustrated by fluid dynamics, the reason why CA parallel computations can be quicker is not purely numerical but is deeply rooted within physics itself..

Computational issues involve different distinct questions that should not be mixed up. “What is the less-greedy model to study such phenomenon?”, “What is the most efficient method to solve this model ?”, or “Is it worth building parallel less versatile computers to perform this task (e.g. climate prediction)?”. These questions about parallel computation and complexity are still currently studied (Machta, 2006); however, available results about these issues already show that CA seem to be a tool worth using and investigating. These issues about complexity and good use of computational resources are quite independent of the much more speculative debates about fundamental physics that we mentioned in section 4.5. As philosophers we should clearly keep debates separate.

6. Conclusion

CA are first and foremost discrete dynamical systems performing parallel computation. Their mathematical properties make up the starting point of any rigorous analysis of their role in modeling and simulation. They explain why CA can be used to perform computation that are significant for physics or other scientific investigation. We have argued that accordingly, CA can be put side by side with calculus, since their formal properties endow them with a remarkable representational capacity. However, we have shown that generalizations about the possibilities of CA for modeling are hardly justified. CA are used in a great variety of cases. Further, in spite of the novelty of CA as modeling tools, some of CA based models, *e.g.* lattice gases, are rooted in traditional physics.

We have also insisted that CA’s computational and representational ability do not make a universal panacea of them for any kind of modeling situation. CA, like PDE, bear complex relations to theories. CA based models, like PDE based models, encapsulated theoretical hypotheses the consequences of which they allow to compute. Such a translation is never a non-problematic one, be it with CA or with PDE. Moreover, questions about model’s tractability occur for CA-based models in the same way as they do for classical models. Parallel computation is not a miraculous for all modeling questions. One virtue of our systematic examination of what is currently done with CA is perhaps to shed a new light on the relationships between modeling and computation.

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